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MEMORANDUM FOR PRS (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)

2 July 1999

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-FY99-0162  
Dr Perkins, "Computational Chemistry and Material Science for Rocket Propulsion"

**Defense S&T Presentation**

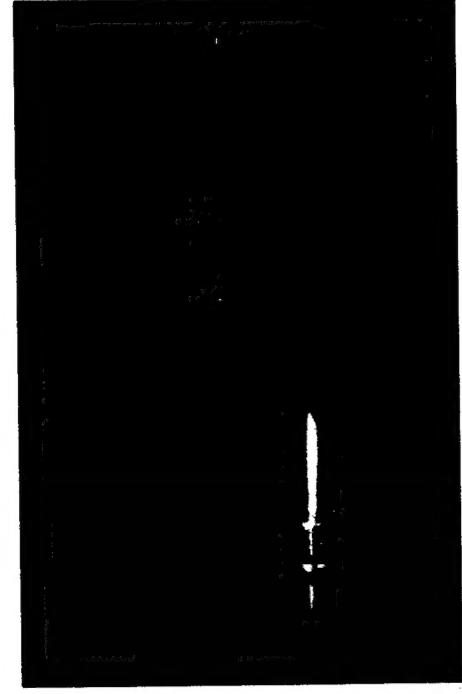
(Statement A)

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# Computational Chemistry and Materials Science for Rocket Propulsion

20021121 014



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# High Performance Computing is **Vital** to Materials Development in Rocket Propulsion!

- Identifies material improvements for liquid engines and solid motors
  - Decide which proposed materials are worthwhile to pursue: Months rather than years!
- Reduces the long process to synthesize new materials.
  - Eliminate unlikely pathways for making a new material



# Approach to Developing Advanced Materials

Employ a synergistic blend of experimental and theoretical techniques derived from the disciplines of chemistry and physics

## Experiments

Exploratory experiments

Identify target compounds

Calculate stability and performance

## Theory & modeling

Develop new synthesis methods

Attempt synthesis on small scale

Calculate possible synthesis routes

Measure properties & compare with predictions

Characterize new materials

Model spectral fingerprints

Optimize synthesis methods

Scale up for formulation and testing



# New Energetic All-Nitrogen Compound

From Chemical and Engineering News, 25 Jan 99

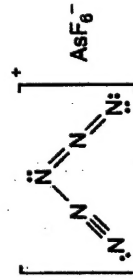
news of the week

## $N_5^+$ CATION MAKES EXPLOSIVE DEBUT

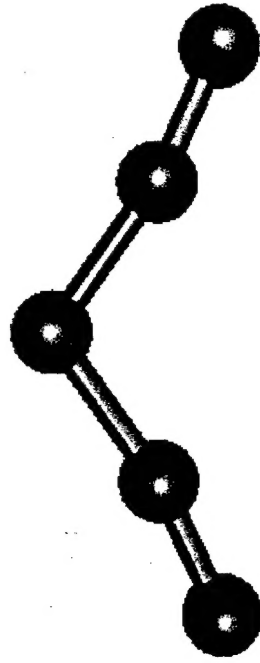
*High-energy ion is first new all-nitrogen species in 100 years*

It wasn't in his abstract, but Karl O. Christe, a chemist who studies high-energy materials at the Air Force Research Laboratory at Edwards Air Force Base in California, had a little something extra to offer last week in his plenary presentation at the American Chemical Society's Winter Fluorine Conference in St. Petersburg Beach, Fla. Along with colleague William W. Wilson, Christe has synthesized and characterized a salt containing the  $N_5^+$  cation. The cation is the first new all-nitrogen species to be synthesized in isolable quantities in more than a century, and only the third ever to be produced.

Although species that contain only ni-



taking," says Gary J. Schrobilgen, a professor of chemistry at McMaster University, Hamilton, Ontario. "This synthesis could only be done in a very few laboratories in the world, and certainly Christe's is one of them." The work is supported by the Air Force Research Laboratory's propulsion directorate as well as by the Defense Advanced Research Projects Agency and the



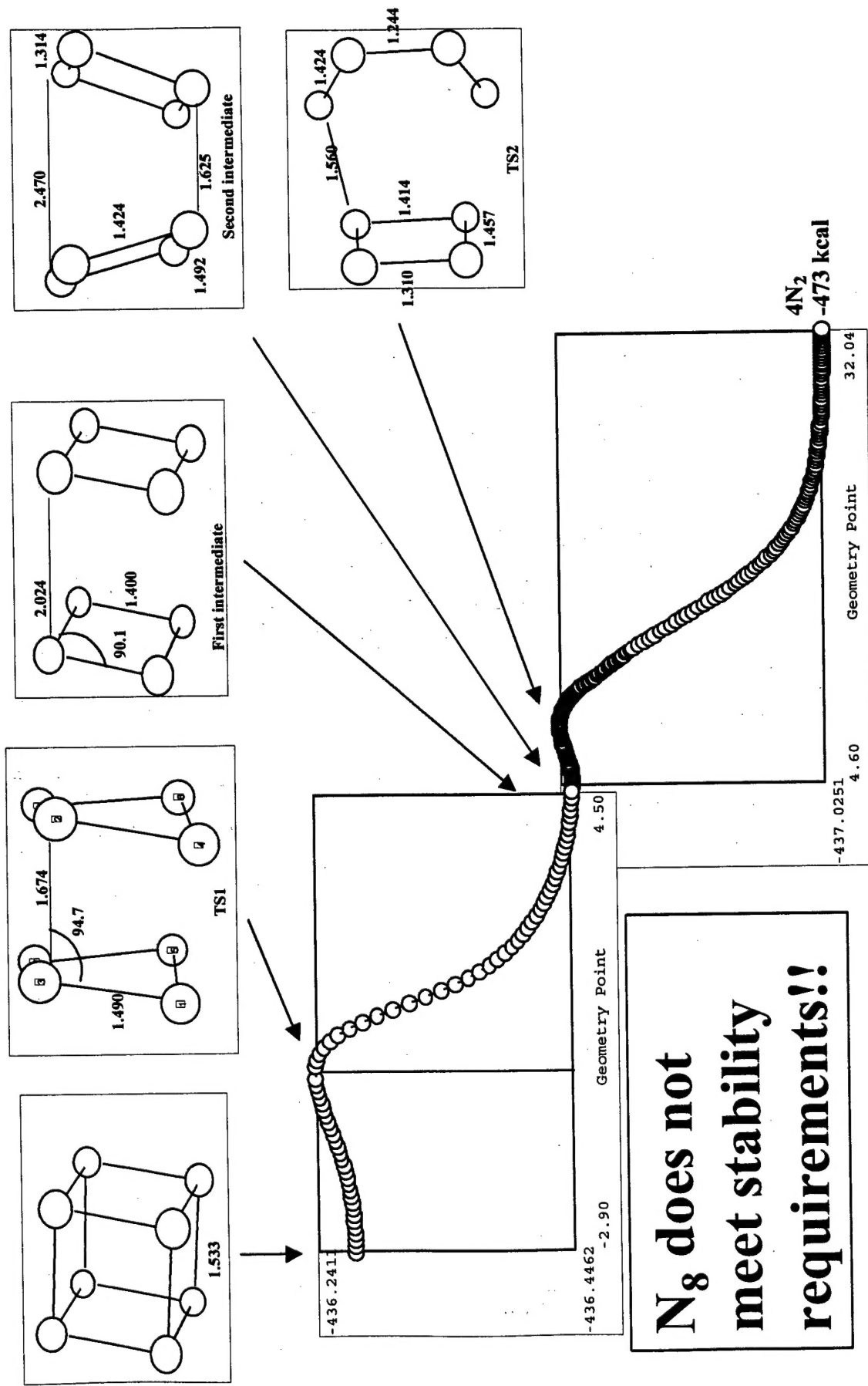
be theoretical chemists who are usually most interested in the new cation. "It's going to be of incredible interest to theoreticians who, perhaps, thought that compounds like this would be too unstable to isolate at all," Strauss says.

The salt is surprisingly stable, considering its huge calculated positive heat of formation of more than 350 kcal per mol, Christe points out. Vibrational spectroscopy and theoretical calculations by his coworkers Jeffrey A. Sheehy and Jerry A. Boatz show the cation to have a V shape in which resonance structures increase its stability.

Christe and his group envision other  $N_5^+$  salts—such as  $N_5^+SbF_6^-$ —that might have even more thermal stability. They also would like to use the cation to pre-

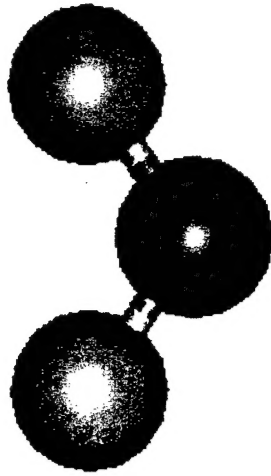


# Evaluation of $N_8$ for stability



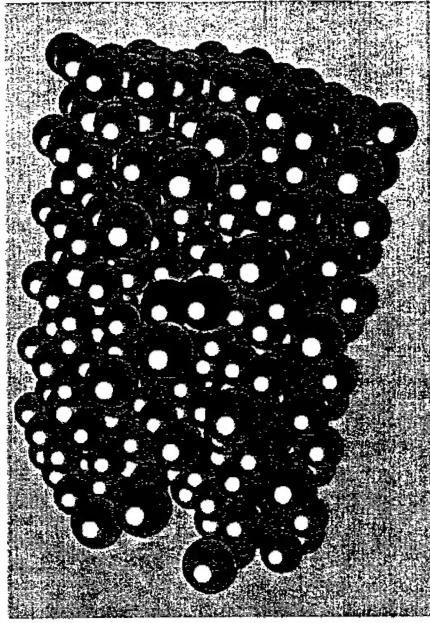


# HPC aids in identifying future propellants



In 1987, a single calculation would take over 1 week.

Software  
&  
Hardware



Software

**GAMESS calculation on  
a workstation: 8 hours!!**

**B in *para*-H<sub>2</sub>: 200 times  
the number of atoms in 5  
weeks on IBM SP!! (This  
would require 4 YEARS on a  
workstation)**

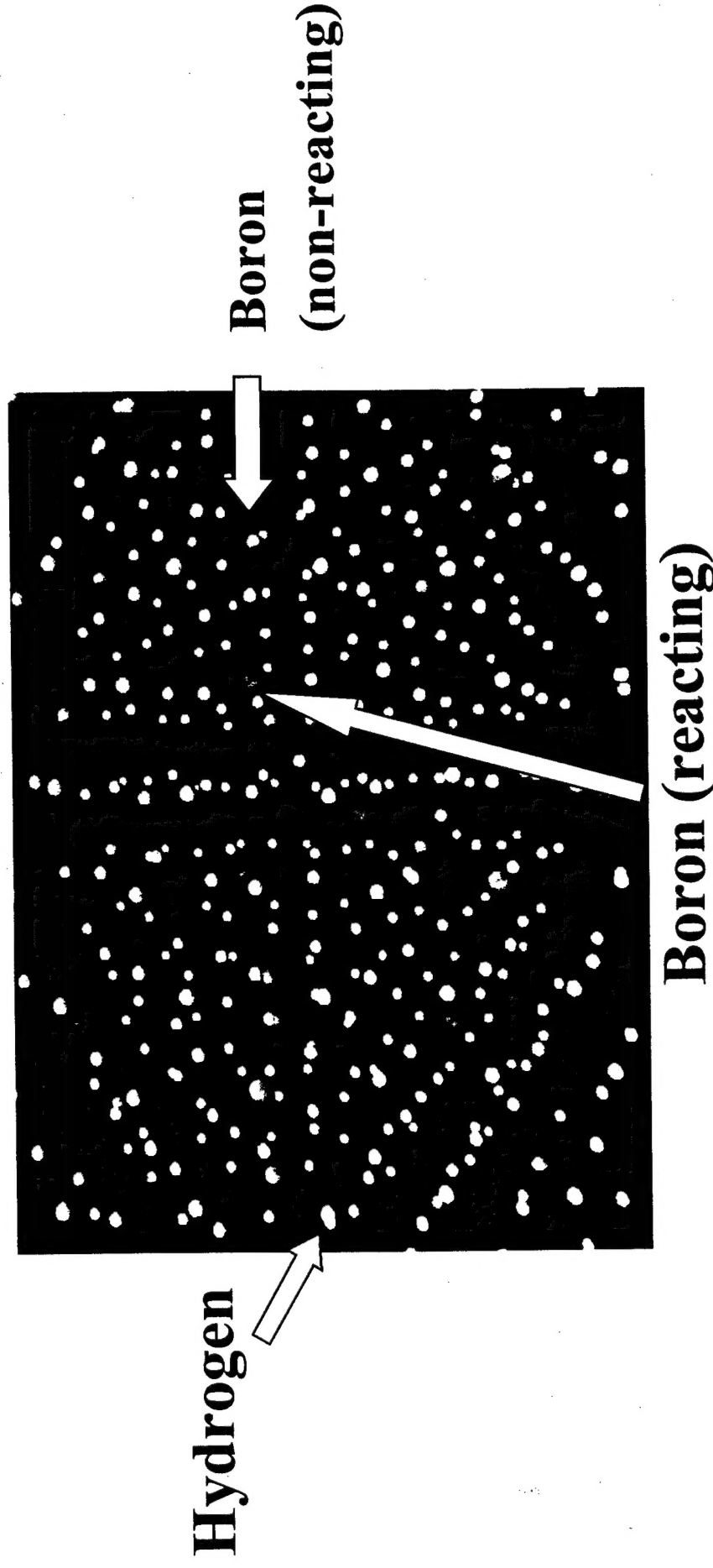




# Future Solid Propellants

6.25% boron atoms in solid *para*-hydrogen

(64 nodes on an IBM SP at Maui - 5 weeks)

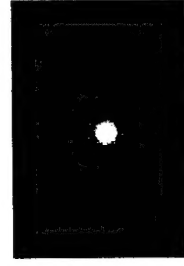


After reaction: Only local recombination of impurities!

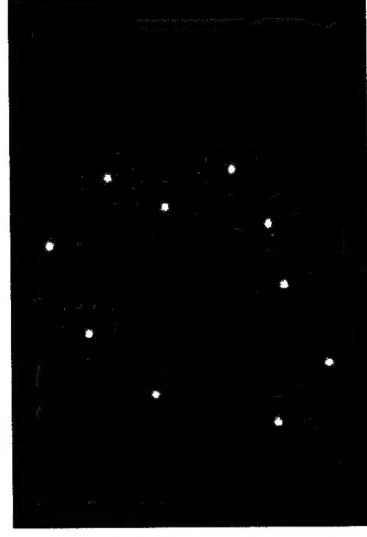


# CMD: Quantum Particles and Classical Dynamics

1. Treat the quantum particles as a “ring” of classical particles

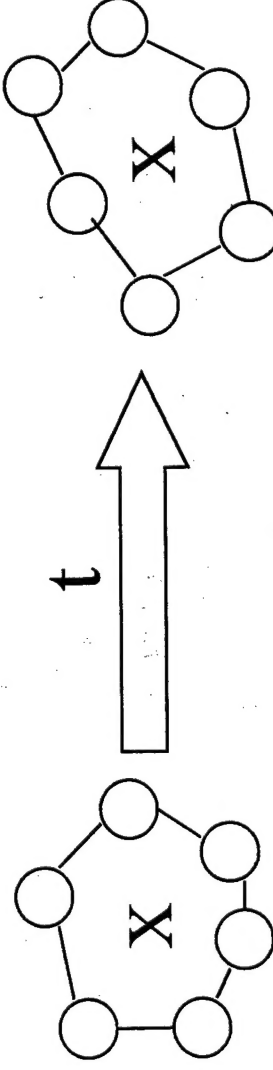


Quantum  $\propto M^N$



Classical  $\propto N$  to  $N^2$

2. The dynamics of the “ring” is calculated for each time step.



$q_c(0)$

$q_c(t)$



# CMD on HPC Architectures

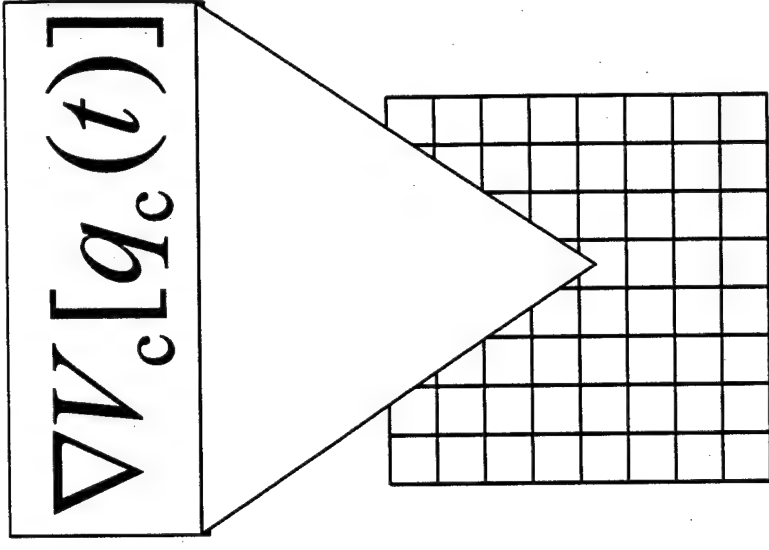
Compute the movement of particles using:

$$m \bullet \frac{d^2 q_c(t)}{dt^2} = -\vec{\nabla} V_c[q_c(t)]$$

where

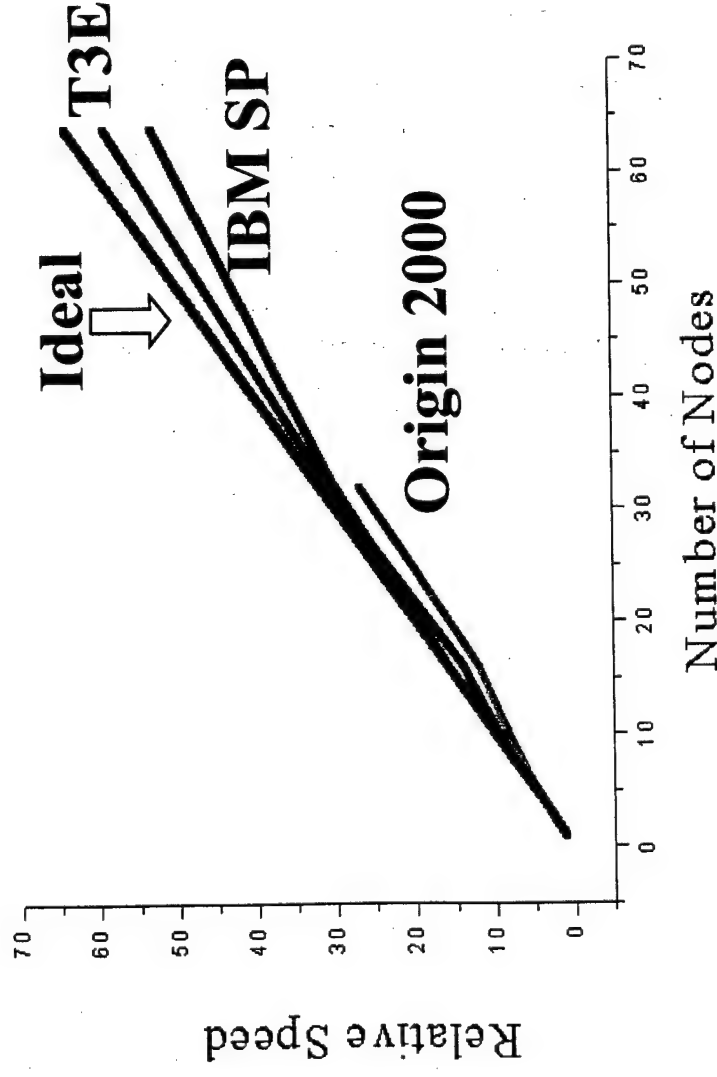
$$V_c(q_c) = -k_B T \ln[\rho_c(q_c)]$$

The largest part of the work is solution of the forces. It is equally balanced onto 64 nodes.





# How does CMD perform on HPC machines?

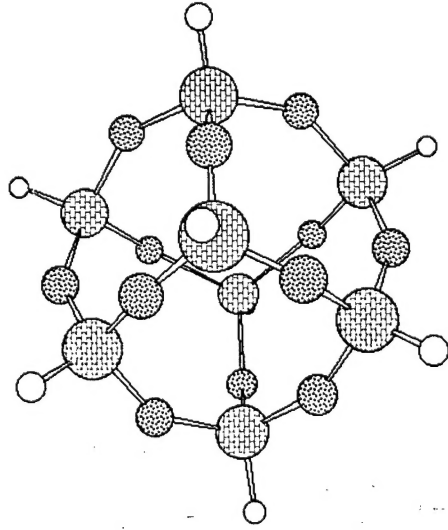


CMD shows different performance curves on the three machines.

Parallel coding is not a “one-size fits all” procedure



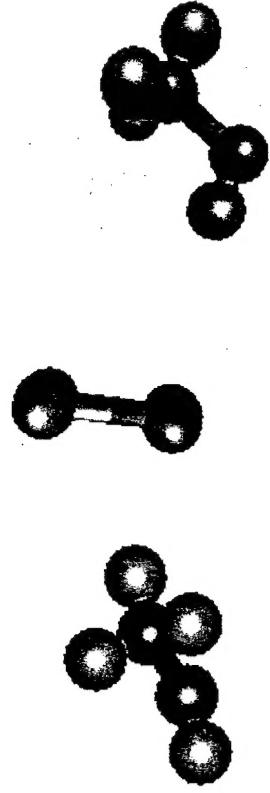
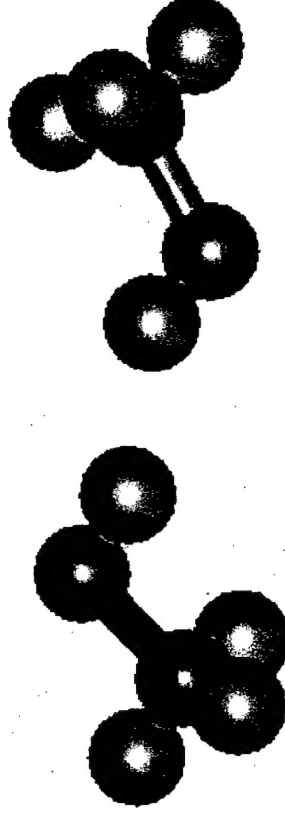
# HPC in Materials Design and Synthesis



Polyhedral  
Oligomeric  
Silsesquioxane  
(POSS)



Significant barrier to  
initial condensation -  
20 kcal/mol

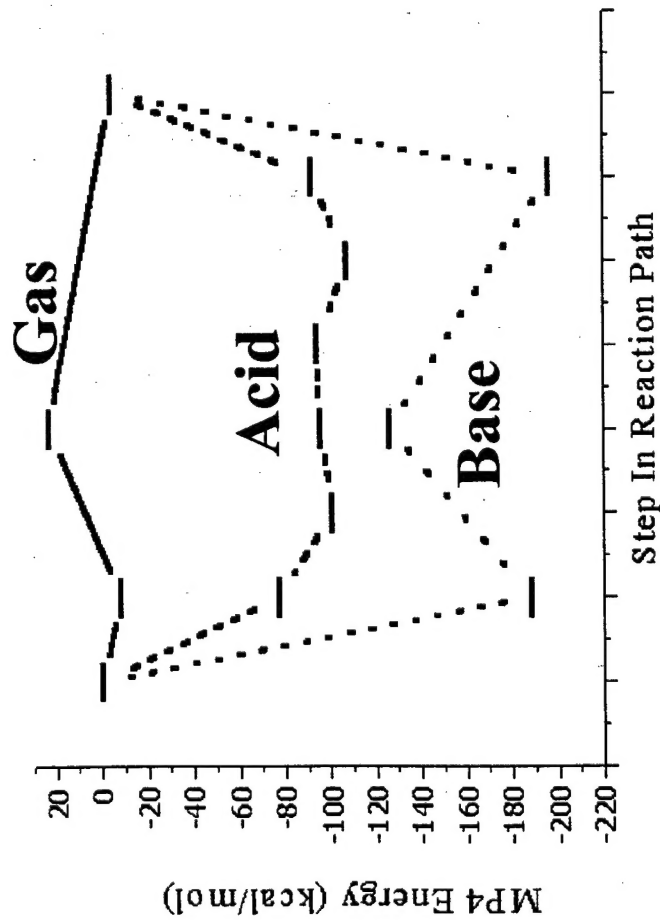


In a basic solution, the  
condensation pathway is  
more favorable!



# Condensation of POSS

- There are different reaction pathways with different liquid environments
- Aids in experimental design to get to end product
- UNABLE to accomplish prior to HPC!!!





# Computational Chemistry and Materials Science - Future Directions

- Simulations of “real” sized systems
  - Material simulations consisting of billions of atoms with a volume of *at least* 1 cubic centimeter
- Dynamic and static simulations that include a quantum effects *without* a significant turnaround time for results
  - Software development that incorporates quantum mechanics in an ingenious manner



# HPC - What has it done for Rocket Propulsion?

- HPC has identified likely candidates ( $N_5^+$ , B in solid H, POSS) and rejected unlikely prospects ( $H_4, N_8$ ) in the AFRL/PR Rocket Propellant and Rocket Component Materials programs
- HPC has identified likely routes to achieve the creation of new rocket materials